The program `Formal_Charges`

Version July 2018, Nebil A. Katcho - ILL

The program `Formal_Charges` is a console utility for converting CIF files to CFL files that allows Bond-Valence Energy Landscapes calculations with the program BondStr. The program is fully based in CrysFML (Crystallographic Fortran 95 Modules Library).

The program needs an input file that can be either a standard CIF file or a CFL file containing just the necessary structural information. The input file can be given as a command-line argument that is the name of the file to be processed. If the file has the extension BUF, the program assumes that the input file contains a list of CFL or CIF files to be processed. In this last case another buffer file is created to be treated by BondStr program.

If the program is invoked without command-line argument it asks for the name of a CIF or CFL file to be treated. Example:

```
c:\Examples_fch>Formal_Charges
              ============================
              ====== FORMAL CHARGES ======
              ============================
    ********************************************
    *  Formal charges from  *.cfl or *.cif files  *
    ********************************************
      (Nebil A. Katcho - ILL, version: July 2018 )

 => Code of the file xx.cfl(cif) (give xx):
```

The use should give a valid code (xx) existing in the current directory. If not the program stops after giving a message:

```
c:\Examples_fch>Formal_Charges
              ============================
              ====== FORMAL CHARGES ======
              ============================
    ********************************************
    *  Formal charges from  *.cfl or *.cif files  *
    ********************************************
      (Nebil A. Katcho - ILL, version: July 2018 )

 => Code of the file xx.cfl(cif) (give xx): qewr
 File: qewr.cfl (or .cif) doesn't exist!
```

The normal way of invoking the program is providing a command-line argument:

```
c:\Examples_fch>Formal_Charges NiFePO5_gen.cif
```

```
            ============================
            ====== FORMAL CHARGES ======
            ============================
    ********************************************
    *  Formal charges from  *.cfl or *.cif files  *
    ********************************************
      (Nebil A. Katcho - ILL, version: July 2018 )

  => Treating the file: NiFePO5_gen.cif          #     1

  Total number of treated files:     1
  CPU-Time:       0.05 seconds
  CPU-Time:       0.00 minutes
```

After running the program a file with extension FCH (in this case `NiFePO5_gen.fch`) is generated containing the results of the treatment. The content of this file is self-explanatory.

The most important use of this utility is for treating many CIF files for generating a buffer file with CFL files containing all the proper information to run Bond-Valence Energy Landscapes calculations using BondStr. An example of this use is given below.

```
C:\Database\CIFs>Formal_Charges buffer_small.buf


            ============================
            ====== FORMAL CHARGES ======
            ============================
    ********************************************
    *  Formal charges from  *.cfl or *.cif files  *
    ********************************************
      (Nebil A. Katcho - ILL, version: July 2018)

  => Treating the file: 10069_gen.cif            #     1
  => Treating the file: 10645_gen.cif            #     2
  => Treating the file: 10669_gen.cif            #     3
  => Treating the file: 10670_gen.cif            #     4
  => Treating the file: 10671_gen.cif            #     5
  => Treating the file: 10693_gen.cif            #     6
  => Treating the file: 11282_gen.cif            #     7
  => Treating the file: 11283_gen.cif            #     8
  => Treating the file: 11284_gen.cif            #     9
  => Treating the file: 11285_gen.cif            #    10

  Total number of treated files:    10
  CPU-Time:       0.23 seconds
  CPU-Time:       0.00 minutes
```

After running Formal_Charges using a buffer file containing the names of CIF files the program creates CFL files and a buffer file (`cfl_buffer.buf`) containing the generated CFL filenames. In our case the content of `cfl_buffer.buf` is:

```
C: \Database\CIFs>more cfl_buffer.buf
10069_gen_fch.cfl
10645_gen_fch.cfl
10669_gen_fch.cfl
10670_gen_fch.cfl
10671_gen_fch.cfl
10693_gen_fch.cfl
11282_gen_fch.cfl
11283_gen_fch.cfl
11284_gen_fch.cfl
11285_gen_fch.cfl
```

Notice that the filenames contain the suffix `_fch` for indicating the origin of the CFL files. The content of the generated CFL file depends on additional arguments provided in the command line. In our case only the name of the buffer file has been provided so the content of the CFL file by default is similar to the following:

```
C:\ Database\CIFs>more 10693_gen_fch.cfl
Title  CFL-file generated from by Formal_Charges.f90
!  Automatically generated CFL file (Write_CFL)
!         a              b              c           alpha           beta            gamma
Cell  5.50400         8.28900         6.11700         90.0000         90.0000         90.0000
!     Space Group #  63
Spgr  C m c m
!      Atom  Type     x/a       y/b      z/c        Biso      Occ    Spin    Charge    Info
Atom      Cr  Cr    0.00000   0.64080  0.25000    0.00000   0.25000   0.00    5.00   # None
Atom      Cr  Cr    0.00000   0.00000  0.00000    0.00000   0.12500   0.00    5.00   # None
Atom      Li  Li    0.00000   0.00000  0.00000    0.00000   0.12500   0.00    1.00   # None
Atom       O  O     0.00000   0.24540  0.96270    0.00000   0.50000   0.00   -2.00   # None
Atom       O  O     0.24320   0.02970  0.25000    0.00000   0.50000   0.00   -2.00   # None

! Bond_STR instructions
! Nx, Ny, Nz, Species, Dmax, Delta(eV):
BVEL    55   83   61 Li+1     10.00    3.00
PERCOLATION   3.5
```

By default the program determines the chemical species that is probably the mobile ionic species in the given chemical compound. The user can change that by adding a second argument in the command line corresponding to the desired ionic species. For instance invoking the program as:

```
C:\Database\CIFs>Formal_Charges buffer_small.buf Na+1
```

Moreover if the user wants to use soft bond-valence parameters in BondStr an argument containing the keyword `SOFTBVS` should be given as in:

```
C:\Database\CIFs>Formal_Charges buffer_small.buf SOFTBVS
```

If both the chemical species and soft BVS parameters are to be used, the chemical species name should be given before the keyword `SOFTBVS` as in:

```
C:\Database\CIFs>Formal_Charges buffer_small.buf Na+1 SOFTBVS
```

The CFL files can be used directly to perform BVEL calculations by BondStr that admits also the buffer file containing CFL files generated by `Formal_Charges`.